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FAX COVER SHEET

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DATE: March 8, 2005
TO: Examiner Kurt Fernstrom
 United States Patent and Trademark Office
FROM: Michelle L. Evans
RE: U.S. Patent Application Serial No. 10/625,358 entitled "NMR Teaching Method and Apparatus"
FAX #: 1-571-273-4422

No. of pages (including this cover sheet): 74

MESSAGE:

Enclosed you will find a substitute specification for the above referenced patent application per your request. I have removed the spectrum illustrations from pages 34, 35, 39, 42 and 43. To provide clarity within the application I have added the text "is incorporated herein by reference" to the first line of each of the spectrum examples. On the modified specification, these additions can be found at page 36, lines 3 and 4; page 37, lines 12 and 13; page 40, lines 23 and 24; and page 43, lines 6 and 7. If you have any additional questions or concerns, please let me know.

As this facsimile is quite long, please call, fax or email to confirm receipt.

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**IN THE UNITED STATES
PATENT AND TRADEMARK OFFICE**

TITLE:

NMR TEACHING METHOD AND APPARATUS

INVENTOR:

JOHN V. McCLUSKY

BACKGROUND OF THE INVENTION

1. Field of The Invention

Applicant's invention relates to a method and apparatus for teaching students the principles of structural analysis using nuclear magnetic resonance (NMR) spectroscopy.

2. Background Information

9 Nuclear magnetic resonance (NMR) spectroscopy is used for the study of
10 molecular structure through measurement of the interaction of an oscillating
11 radio-frequency electromagnetic field with a collection of nuclei immersed in a
12 strong external magnetic field. These nuclei are parts of the atoms that are
13 assembled into these molecules.

Once the NMR spectrum is obtained, the determination of the unknown structure is based on three requirements indicated on the spectrum. These three requirements are integration, splitting due to spin-spin coupling, and chemical shift. Each anticipated chemical fragment is determined from the chemical shift on the spectrum. Chemically different hydrogens in a molecule do not experience the same magnetic field. Electrons shield the nucleus; thereby reducing the effective magnetic field and requiring energy of a lower frequency to cause resonance. On the other hand, when electrons are withdrawn from a nucleus, the nucleus is deshielded and feels a stronger

1 magnetic field requiring more energy (higher frequency) to cause resonance.
2 Thus, the NMR spectrum can provide information about a hydrogen's electronic
3 environment. Generally, hydrogens bound to carbons attached to electron
4 withdrawing groups tend to resonate at higher frequencies (more downfield, to
5 the left of the spectrum) from TMS, tetramethylsilane, a common NMR
6 standard. The position of where a particular hydrogen atom resonates relative
7 to TMS is called the chemical shift.

8 Integration is the second item that can be determined from an NMR
9 spectrum. For the integration, the area under the NMR resonance is
10 proportional to the number of hydrogens which contribute to that resonance.
11 In this way, by measuring or integrating the number of different NMR
12 resonances, information concerning the relative number of chemically distinct
13 hydrogens can be obtained. Experimentally, the integrals often appear as a
14 line over the NMR spectrum. Integration only gives information on the relative
15 number of different hydrogens on the represented chemical fragment, not the
16 absolute number.

17 The last item of information that can be determined from the NMR
18 spectrum is splitting. The spectrum provides information on how many
19 hydrogen neighbors exist for a particular hydrogen or group of equivalent
20 hydrogens. In general, an NMR resonance will be split into $N+1$ peaks where N
21 is the number of hydrogens on the adjacent atom or atoms. If there are no
22 hydrogens on the adjacent atoms, then the resonance will remain a single

1 peak, a singlet. If there is one hydrogen on the adjacent atoms, the resonance
2 will be split into two peaks of equal size to form a doublet. Two hydrogens on
3 the adjacent atoms will split the resonance into three peaks with a ratio of
4 1:2:1 being a triplet. If there are three hydrogens on the adjacent atoms, the
5 resonance will split into four peaks with an area in the ratio of 1:3:3:1 forming
6 a quartet.

7 When a student is first introduced to these concepts in an organic
8 chemistry course, he or she does not typically have difficulty determining the
9 identity of an unknown molecule as long as the molecule remains fairly simple,
10 such as a molecule having only a few carbons. However, as the molecules
11 become larger and multiply branched, structural determination by the student
12 becomes quite difficult if not impossible.

13 Every full year organic chemistry text includes a chapter or half a
14 chapter on NMR spectroscopy. Subsequent chapters then include practice
15 problems involving NMR interpretation. NMR in these texts is taught the same
16 way. First the authors start with a molecule and explain its spectrum. This is
17 done for several molecules pointing out the chemical shifts, integration and
18 splitting patterns. Several texts point out common patterns, but most leave it
19 to the students to figure out how to go from the spectrum to the molecule.
20 This is a much more difficult process. In some texts, some simple rules are
21 given such as (1) count the number of signals which is equal to the number of

1 types of hydrogens, (2) figure out the chemical fragments from the chemical
2 shifts, (3) and solve the problem.

3 While this can work for simple molecules it is virtually guaranteed to fail
4 for more complex spectra. Unfortunately, there are currently no "hands-on"
5 educational tools available to assist students with molecular structure
6 identification from NMR spectra, particularly complex spectra. The present
7 invention satisfies this need for a "hands-on" NMR educational tool which can
8 assist students in NMR structural analysis.

9 SUMMARY OF THE INVENTION

10 More specifically, the present invention provides an NMR teaching
11 method and apparatus incorporating a series of pieces that represent chemical
12 functional groups such as methine, methylene, methyl, amine, alkene,
13 aromatic ring, alcohol, thiol, aldehyde, ketone, and halide groups. Each piece
14 typically has the number of sides that corresponds to the number of bonds
15 present around the central atom. Bonds to hydrogen are preferably curved
16 while bonding sides are flat.

17 The presence of concavities and convex tabs on the bonding sides
18 indicates bonding of the respective piece to a mating piece that causes
19 splitting of the NMR peak. The shape of concavities on each piece is indicative
20 of the number of hydrogens on the respective piece while the shape of the
21 convex tab of the respective piece is indicative of the number of hydrogens on
22 the mating piece.

When presented with an NMR spectrum, a student user can select the necessary pieces of the present invention by using the chemical shift, integration, and splitting data from the spectrum. Once the pieces are selected, the student user can then assemble the pieces to determine the identity of the unknown molecule in the NMR spectrum. This tool and method can be used with not only small unknown molecules but large molecules as well, thus permitting the student user to learn NMR structural identification in a simple and relaxed manner.

BRIEF DESCRIPTION OF THE DRAWINGS

10 Fig. 1 is a top view of the methine CH pieces of the present invention.

11 Fig. 2 is a top view of the methylene CH_2 pieces of the present
12 invention.

13 Fig. 3 is a top view of the methyl pieces CH_3 of the present invention.

14 Fig. 4 is a top view of the quaternary carbon piece of the present
15 invention.

16 Fig. 5 is a top view of the alcohol and thiol group pieces of the present
17 invention.

18 Fig. 6 is a top view of the amine pieces of the present invention.

Fig. 7 is a top view of the alkene pieces of the present invention.

20 Fig. 8a is a top view of the benzene pieces of the present invention.

Fig. 8b is a top view of the aromatic pieces of the present invention.

Fig. 9 is a top view of the aldehyde pieces of the present invention.

1 Fig. 10 is a top view of the ketone, ether, and ester pieces of the
2 present invention.

3 Fig. 11 is a top view of the halide piece of the present invention.

4 Fig. 12 is a top view of another embodiment of the present invention
5 showing a base methyl piece with interchangeable tabs.

6 Fig. 13 is a perspective view of another embodiment of the present
7 invention showing a base methyl piece with a single rotating tab member.

8 Fig. 14A is a perspective view of the preferred embodiment of the
9 present invention used to make a first attempt at constructing a molecule.

10 Fig. 14B is a perspective view of the preferred embodiment of the
11 present invention used to make a second attempt at constructing a molecule.

12

13 DETAILED DESCRIPTION OF THE PREFERRED EMBODIMENT

14 Figs. 1-13 illustrate various pieces that are currently available in the
15 preferred embodiment of the present invention; however, several additional
16 pieces are anticipated to cover additional chemical fragments. Duplicates of
17 pieces are obviously possible in the preferred embodiment and some duplicate
18 pieces have been included to emphasize this. In addition, mirror images of
19 pieces are also possible as are pieces having the convex tab and concavity
20 reversed on each respective side. The pieces can be provided with the sides in
21 a different order such as in the case for the methine pieces. The NMR splitting

1 side and non-splitting side can also be reversed. Some examples of this are
2 provided, but are by no means inclusive of all possibilities.

3 Each piece of the present invention typically has the number of sides
4 corresponding to the number of bonds present around the central atom. Bonds
5 to hydrogen are preferably curved but can be any shape which indicates no
6 further pieces bind to that respective side. Bonding sides are flat being either
7 with or without both concavities and convex tabs. The presence of concavities
8 and convex tabs on the piece indicates bonding is to be made to an atom(s) or
9 group(s) that causes splitting of the NMR peak, whereas a piece not having
10 concavities and convex tabs is indicative of bonding to an atom(s) or group(s)
11 that does not cause splitting. The shape of the concavities indicates the
12 number of splitting hydrogens on that chosen piece, while the shape of the
13 convex tabs indicates the number of hydrogens on the piece to which the
14 chosen piece is to be bonded. All convex tabs interlock with the respective
15 concavities present on the adjoining piece. No convex tabs or concavities are
16 present on the curved hydrogen sides. Each side of the pieces is the same
17 length unless otherwise indicated.

18 While the preferred embodiment discusses the use of concavities and
19 convex tabs, any design can be utilized in place of the concavities and convex
20 tabs as long as the substitute design for the concavities represents the number
21 of splitting hydrogens on the chosen piece and the substitute design for the
22 convex tabs represents the number of hydrogens on the piece to which the

1 chosen piece is to be bonded. In this case, the design can be color, letters,
2 numbers, or an ornamental pattern either written/typed/drawn on the pieces
3 or as a cutout on the pieces, such as, but not limited to curves or magnetic
4 fields.

5 Fig. 1 shows a top view of the methine CH pieces 102-150 of the present
6 invention. These pieces have three bonding sides 152 and one curved hydrogen
7 side 154. One piece 102 is present without concavities and convex tabs and
8 would be bonded to only an atom(s) or group(s) that does not cause observable
9 splitting of the NMR peak. The remaining pieces 103-150 contain concavities
10 and convex tabs. Table 1 illustrates the number of variations possible for the
11 methine pieces

1 103-150.

Piece Number	Number of Flat Sides with No Tabs	Number of Sides with Methine Convex Tab	Number of Sides with Methylene Convex Tab	Number of Sides with Methyl Convex Tab
102	3	0	0	0
107	2	1	0	0
112	2	0	1	0
110	2	0	0	1
150/146	1	2	0	0
116/120	1	0	2	0
124/122	1	0	0	2
136/142	1	1	1	0
138/130	1	1	0	1
126/104	1	0	1	1
103	0	3	0	0
118	0	0	3	0
105	0	0	0	3
128	0	1	1	1
148	0	2	1	0
144	0	2	0	1
134	0	1	2	0
132/140	0	1	0	2
106/108	0	0	1	2
114	0	0	2	1

2

3 Table 1: Methine Pieces

4 There is only one type of concavity 156 present on these pieces 103-150
 5 since the concavity represents the number of splitting hydrogens on these
 6 pieces 103-150. The concavity 156 present on pieces 103-150 has preferably
 7 three flat inset sides generally in the shape of a square; however, any shape
 8 can be used as long as it is consistent on all methine pieces 103-150 and the
 9 convex tabs on all mating pieces.

1 The convex tabs on pieces 103-150 vary depending on the atom(s) or
2 group(s) to which the pieces 103-150 can be bound. Where pieces 103-150 are
3 to be bound to a mating piece representing a group having one hydrogen, such
4 as another methine piece, the convex tab 158 will preferably have three flat
5 sides generally in the shape of a square; however, any shape can be used as
6 long as it is consistent for the concavity of the mating piece. Pieces 103, 107,
7 and 128-150 are capable of being bound to a mating piece representing a group
8 having one hydrogen, such as another methine piece 103-150. Pieces 107 and
9 128-142 are capable of binding to only one mating piece representing a group
10 having one hydrogen; however, pieces 144-150 are capable of binding to two
11 mating pieces representing a group having one hydrogen. Piece 103 can bind
12 three mating pieces representing a group having one hydrogen.

13 Where pieces 103-150 are to be bound to a mating piece representing a
14 group having two hydrogens, such as a methylene CH_2 piece, the convex tab
15 160 is preferably shaped as an equilateral triangle, but can be any shape as
16 long as it is consistent for the concavity of the mating piece. Pieces 104, 106,
17 108, 112, 114, 116, 118, 120, 126, 128, 134, 136, 142, and 148 all have convex
18 tabs 160 and are capable of binding to at least one mating piece representing a
19 group having two hydrogens. Pieces 104, 106, 108, 112, 126, 128, 136, 142 and
20 148 are capable of binding to only one mating piece representing a group
21 having two hydrogens. Pieces 114, 116, 120, and 134 can bind to as many as

1 two mating pieces representing a group having two hydrogens while piece 118
2 can bind to three mating pieces representing a group having two hydrogens.

3 Pieces 103-150 can also be bound to a mating piece representing a group
4 having three hydrogens, such as a methyl CH₃ piece. Where a piece 103-150 is
5 bound to a mating piece representing a group having three hydrogens, the
6 convex tab 162 is preferably shaped as a diamond; however, any shape can be
7 used as long as it is consistent with the concavity of the mating piece. Pieces
8 104, 105, 106, 108, 110, 114, 122, 124, 126, 128, 130, 132, 138, 140, and 144
9 have convex tabs 162 that can bind to mating pieces representing a group
10 having three hydrogens. Pieces 104, 110, 114, 126, 128, 130, 138, and 144 can
11 bind to one mating piece representing a group having three hydrogens while
12 pieces 106, 108, 122, 124, 132, and 140 are capable of binding to as many as
13 two mating pieces representing a group having three hydrogens. Piece 105 can
14 bind to three mating pieces representing a group having three hydrogens.

15 Fig. 2 is a top view of the methylene CH₂ pieces 164 -200 of the present
16 invention. These pieces have two bonding sides 202 and two curved hydrogen
17 sides 204. One piece 164 is present without concavities and convex tabs and
18 can be bonded to an atom(s) or group(s) that does not cause observable
19 splitting of the NMR peak. The remaining pieces 165-200 contain concavities
20 and convex tabs. Table 2 illustrates the number of variations possible for the
21 methylene pieces 165-200.

Piece Number	Number of Flat Sides with No Tabs	Number of Sides with Methine Convex Tab	Number of Sides with Methylene Convex Tab	Number of Sides with Methyl Convex Tab
164	2	0	0	0
174	1	1	0	0
180/198	1	0	1	0
178/172/170	1	0	0	1
186/184	0	2	0	0
166/196/168	0	0	2	0
165	0	0	0	2
176/182	0	1	1	0
188/200	0	1	0	1
192/190/194	0	0	1	1

1

2 Table 2: Methylene Pieces

3 There is only one type of concavity 206 present on methylene pieces

4 165-200. This concavity 206 is preferably in the shape of an equilateral

5 triangle; however, any shape can be used as long as it is consistent on all

6 methylene pieces 165-200 and the convex tabs on all mating pieces.

7 The convex tabs on pieces 165-200 vary depending on the atom(s) or

8 group(s) to which they are bound. The convex tab 208 will preferably have

9 three flat sides generally in the shape of a square where pieces 165-200 are

10 bound to a mating piece representing a group having one hydrogen, such as a

11 methine piece. However, the shape of convex tab 208 can vary as long as the

12 shape used is consistent with the concavity of the mating piece. Pieces 174,

13 176, 182, 188, and 200 can bind to a mating piece representing an atom(s) or

14 group(s) having one hydrogen while pieces 184 and 186 are capable of binding

15 two mating pieces representing an atom(s) or group(s) having one hydrogen.

1 Where pieces 165-200 are bound to mating piece representing a group
2 having two hydrogens, such as another methylene CH_2 piece, the convex tab
3 210 is preferably shaped as an equilateral triangle, but can be any shape as
4 long as it is consistent with the concavity of the mating piece. Pieces 166, 168,
5 176, 180, 182, 190, 192, 194, 196, and 198 have convex tabs 210 that are
6 capable of binding to at least one mating piece representing a group having
7 two hydrogens. Pieces 176, 180, 182, 190, 192, 194, and 198 can bind only one
8 mating piece representing a group having two hydrogens while pieces 166, 168,
9 and 196 can bind as many as two mating pieces representing a group having
10 two hydrogens.

11 Methylene pieces 165-200 can also be bound to a mating piece
12 representing a group having three hydrogens, such as methyl CH_3 piece.
13 Where a methylene piece 165-200 is bound to a mating piece representing a
14 group having three hydrogens, the convex tab 212 is preferably shaped as a
15 diamond; however, any shape can be used as long as it is consistent with the
16 concavity of the mating piece. Pieces 170, 172, 178, 188, 190, 192, 194, and
17 200 have a convex tab 212 that can bind to mating pieces representing a group
18 having three hydrogens and can bind to these mating pieces in one location.
19 Piece 165 can bind to a mating piece representing a group having three
20 hydrogens in two locations.

21 In Fig. 3 a top view of the methyl pieces CH_3 214-228 of the present
22 invention is shown. These pieces have one bonding side 230 and three curved

1 hydrogen sides 232. Two pieces 214 and 216 are present without concavities
2 and convex tabs and would be bonded to an atom(s) or group(s) that does not
3 cause splitting of the NMR peak. The remaining pieces 218-228 contain
4 concavities and convex tabs. Table 3 illustrates the number of variations
5 possible for the methyl pieces.

Piece Number	Number of Flat Sides with No Tabs	Number of Sides with Methine Convex Tab	Number of Sides with Methylene Convex Tab	Number of Sides with Methyl Convex Tab
214/216	1	0	0	0
218	0	1	0	0
220/224/222/228	0	0	1	0

6

7 Table 3: Methyl Pieces

8 There is only one type of concavity 234 present on pieces 218-228 which
9 is preferably in the shape of a diamond; however, any shape can be used as
10 long as it is consistent on all methyl pieces 218-228 and the convex tabs of all
11 mating pieces.

12 The convex tabs on pieces 218-228 vary depending on the atom(s) or
13 group(s) to which the pieces 218-228 are bound. Where pieces 218-228 are
14 bound to a mating piece representing a group having one hydrogen, such as a
15 methine piece, the convex tab 236 will preferably have three flat sides
16 generally in the shape of a square; however, any shape can be used as long as
17 it is consistent for the concavity of the mating piece. Piece 218 is capable of
18 binding to one mating piece representing a group having one hydrogen.

1 Where methyl pieces 218-228 are bound to a mating piece representing a
2 group having two hydrogens, such as a methylene piece, the convex tab 238 is
3 preferably shaped as an equilateral triangle, but can be any shape as long as it
4 is consistent for the concavity of the mating piece. Pieces 220-228 have
5 convex tab 238 and are capable of binding to one mating piece representing a
6 group having two hydrogens.

7 A methyl piece having a diamond shaped convex tab that can bind to a
8 mating piece representing a group having three hydrogens is not present in the
9 invention as it represents ethane which gives a singlet on the NMR spectrum.

10 Fig. 4 shows a top view of the quaternary carbon piece 250 of the
11 present invention. This piece 250 has four flat bonding sides 251 without any
12 concavities or convex tabs.

13 Fig. 5 is a top view of the alcohol and thiol group pieces 252-258 of the
14 present invention. These pieces have one bonding side 260 with the remainder
15 of the piece being preferably rounded; however, any shape is possible for this
16 remainder side as long as it is shaped so that no other connections are possible.
17 One piece 252 is present without concavities and convex tabs and would be
18 bonded to an atom(s) or group(s) in which splitting is not observed. The
19 remaining pieces 254-258 contain concavities and convex tabs.

20 The concavity present on pieces 254-258 has preferably three flat inset
21 sides generally in the shape of a square identical to the concavity mentioned
22 for the methine pieces 103-150; however, any shape can be used as long as it is

1 consistent on all alcohol and thiol group pieces 254-258 and with the convex
2 tabs of all mating pieces such as, but not limited to, 208, 158 and 236.

3 The convex tabs vary depending on the atom(s) or group(s) to which the
4 pieces are bound. Piece 254 has a convex tab 253 preferably having three flat
5 sides generally in the shape of a square; however, any shape can be used as
6 long as it is consistent for the concavity of the mating piece. In this case, the
7 mating piece would be representative of a group having one hydrogen, such as
8 a methine piece. Piece 256 has a convex tab 255 preferably being in the shape
9 of an equilateral triangle, but can be any shape as long as it is consistent for
10 the concavity of the mating piece. In this case, the mating piece would be
11 representative of a group having two hydrogens, such as a methylene piece.
12 And piece 258 has a convex tab 257 preferably being in the shape of a
13 diamond, but can be any shape as long as it is consistent for the concavity of
14 the mating piece. In this case, the mating piece is representative of a group
15 having three hydrogens, such as a methyl piece.

16 In Fig. 6 a top view of the amine pieces 260 - 290, 510, 512 and 514 of
17 the present invention is shown. The quaternary amines are pieces 260, 510,
18 512 and 514. Piece 260 has four bonding sides 292. Piece 510 has one bonding
19 side 292 and three curved hydrogen sides 511. Piece 510 is present without
20 concavities and convex tabs and would be bonded to an atom(s) or group(s)
21 that does not cause observable splitting of the NMR peak. Piece 510 can be

1 modified to include the concavities and convex tabs previously discussed for
2 the methyl pieces on the bonding side 292.

3 For piece 512 there are two bonding sides 292 and two curved hydrogen
4 sides 511. This piece 512 is present without concavities and convex tabs and
5 would be bound to an atom(s) or group(s) that does not cause observable
6 splitting of the NMR peak. Piece 512 can be modified to include the
7 concavities and convex tabs previously discussed for the methylene pieces on
8 the bonding sides 292.

9 Piece 514 has three bonding sides 292 and one curved hydrogen side 511.
10 Piece 514 is present without concavities and convex tabs and would be bonded
11 to an atom(s) or group(s) that does not cause observable splitting of the NMR
12 peak. Piece 514 can be modified to include the concavities and convex tabs
13 previously discussed for the methine pieces on the bonding sides 292.

14 The remaining amine pieces 262-290 have three sides and have the basic
15 shape of an equilateral triangle. Piece 262, representative of a tertiary amine,
16 has three bonding sides 294 without concavities and convex tabs and therefore
17 would be bonded to a similar flat side since this nitrogen has no hydrogen to
18 split its neighbor group.

19 Pieces 264-282, representative of secondary amines, contain two
20 bonding sides 294 and one curved hydrogen side 308. Piece 264 is present
21 without concavities and convex tabs and would be bonded to atom(s) or
22 group(s) in which no splitting is observed. The remaining pieces 266-282 have

1 concavities and convex tabs. Table 4 illustrates the number of variations
2 possible for these amine
3 pieces.

4

5

6

Piece Number	Number of Flat Sides with No Tabs	Number of Sides with Square Convex Tab	Number of Sides with Triangle Convex Tab	Number of Sides with Diamond Convex Tab
264	2	0	0	0
280	1	1	0	0
282	1	0	1	0
276	1	0	0	1
270	0	2	0	0
272	0	0	2	0
278	0	0	0	2
274	0	1	1	0
268	0	1	0	1
266	0	0	1	1

7

8 Table 4: Secondary Amine Pieces

9 There is only one type of concavity 298 present on these secondary
10 amine pieces 266-282 since the concavity represents the number of splitting
11 hydrogens on the pieces. The concavity 298 present on these pieces has
12 preferably three flat inset sides generally in the shape of a square; however,
13 any shape can be used as long as it is consistent on all secondary amine pieces
14 266-282 as well as with the convex tabs of all mating pieces.

1 The convex tabs vary on pieces 266-282 depending on the atom(s) or
2 group(s) to which the piece can be bound. When the atom(s) or group(s) to
3 which pieces 266-282 are bound has one hydrogen, the convex tab 300 will
4 preferably have three flat sides generally in the shape of a square; however,
5 any shape can be used as long as it is consistent for the concavity of the mating
6 piece. Pieces 268, 270, 274, and 280 are all capable of binding to a piece
7 representing atom(s) or group(s) with one hydrogen. Pieces 268, 274, and 280
8 can bind only one piece representing atom(s) or group(s) with one hydrogen;
9 whereas piece 270 can bond to two such pieces.

10 When the mating piece to which pieces 266-282 are bound represents a
11 group having two hydrogens, the convex tab 302 is preferably shaped as an
12 equilateral triangle; however, any shape can be used as long as it is consistent
13 for the concavity of the mating piece. Pieces 266, 272, 274 and 282 are
14 capable of bonding to a piece representing atom(s) or group(s) with two
15 hydrogens. Pieces 266, 274, and 282 are capable of bonding to only one piece
16 representing atom(s) or group(s) with two hydrogens with piece 272 being
17 capable of binding to two such pieces.

18 When the mating piece to which piece 266-282 is bound has three
19 hydrogens, the convex tab 304 is preferably shaped as a diamond; however,
20 any shape can be used as long as it is consistent for the concavity of the mating
21 piece. Pieces 266, 268, 276 and 278 are capable of bonding to a piece
22 representing atom(s) or group(s) with three hydrogens. Pieces 266, 268, and

1 276 are capable of bonding to only one piece representing atom(s) or group(s)
2 with three hydrogens and piece 278 is capable of bonding two such pieces.

3 Pieces 284-290, representing primary amines, have one bonding side 306
4 and two curved hydrogen sides 308. One piece 284 is present without
5 concavities and convex tabs and would be bonded to an atom(s) or group(s) in
6 which splitting of the NMR peak is not observed. The remaining pieces 236-290
7 contain concavities and convex tabs. Table 5 illustrates the number of
8 variations possible for these
9 pieces.

Piece Number	Number of Flat Sides with No Tabs	Number of Sides with Square Convex Tab	Number of Sides with Triangle Convex Tab	Number of Sides with Diamond Convex Tab
284	1	0	0	0
290	0	1	0	0
286	0	0	1	0
288	0	0	0	1

10

11 Table 5: Primary Amine Pieces

12 There is only one type of concavity 310 present on these pieces 236-290
13 since the concavity represents the number of splitting hydrogens on these
14 pieces. The concavity 310 present on pieces 286-290 is preferably shaped as an
15 equilateral triangle; however, any shape can be used as long as it is consistent
16 for all primary amine pieces 286-290 and with the convex tabs of all mating
17 pieces, including, but not limited to convex tabs 210, 238, 255, 160, 406, 349,
18 302, 314, 505, 517, 604, and 717.

1 The convex tabs on pieces 286-290 vary depending on the atom(s) or
2 group(s) to which the pieces 286-290 are bound. Piece 290 is designed to bind
3 to a piece representing atom(s) or group(s) having one splitting hydrogen.
4 Piece 290 has a convex tab 312 having preferably three flat sides generally in
5 the shape of a square; however, any shape can be used as long as it is
6 consistent for the concavity of the mating piece.

7 Piece 286 is designed to bind to a piece representing atom(s) or group(s)
8 having two splitting hydrogens. This piece 286 has a convex tab 314 being
9 generally in the shape of an equilateral triangle; however, any shape can be
10 used as long as it is consistent for the concavity of the mating piece.

11 The remaining piece 288 is designed to bond to a piece representing
12 atom(s) or group(s) having three hydrogens. Piece 288 has a convex tab 314
13 preferably shaped as a diamond; however, any shape can be used as long as it
14 is consistent for the concavity of the mating piece.

15 Fig. 7 is a top view of the alkene pieces 320-342, 502, 504, 506, 516, 518
16 and 520 of the present invention. The alkene pieces 320-342, 502, 504, 506,
17 516, 518 and 520 are complex in that the geminal hydrogens can appear at
18 different locations in the NMR spectrum; therefore, each piece does not
19 necessarily represent a single carbon with all its hydrogens. Pieces 320-342,
20 516, 518, and 520 have at least one flat bonding side 344 and may or may not
21 have a curved hydrogen side 346. Pieces 338 and 340 are shaped as diamonds
22 with all sides of equal length and represent alkene carbons without hydrogens.

1 These pieces 338 and 340 are present without concavities and convex tabs
 2 which indicates that these pieces do not cause observable splitting of their
 3 neighbor, so would be attached at a matching flat bonding side. Pieces 320-
 4 342, 502, 504, 506, 516, 518 and 520 permit assembly of mono-, di-, tri- and
 5 tetra-substituted alkenes.

6 Pieces 320-336, 516, 518 and 520 are shaped as isosceles triangles with
 7 each piece representing one of the alkene hydrogens. These pieces have at
 8 least two flat bonding sides 344 and may or may not have one curved hydrogen
 9 side 346. Piece 520 has two flat bonding sides 344 and one curved hydrcgen
 10 side 346. This piece does not have concavities and convex tabs which indicates
 11 this piece does not cause observable splitting of its neighbor. Table 6
 12 illustrates the number of variations possible for the remaining alkene pieces
 13 320-336, 516, 518 and 520.

14

Piece Number	Number of Curved Hydrogen Sides	Number of Flat Sides with No Tabs	Number of Sides with Square Convex Tab	Number of Sides with Triangle Convex Tab	Number of Sides with Diamond Convex Tab
334/336	1	1	1	0	0
324	1	0	1	1	0
326	1	0	1	0	1
328/332	1	0	2	0	0
323	0	0	3	0	0
322	0	0	2	1	0
320	0	0	2	0	1
330	0	1	2	0	0
516	1	1	0	1	0
518	1	1	0	0	1
520	1	2	0	0	0

15

1 Table 6: Alkene Pieces

2 There is only one type of concavity 348 present on these remaining
3 alkene pieces 320-336, 516, 518 and 520 since the concavity represents the
4 number of splitting hydrogens on these pieces. The concavity 348 present on
5 pieces 320-336, 516, 518 and 520 has preferably three flat sides generally in
6 the shape of a square; however, any shape can be used as long as it is
7 consistent for these pieces and with the convex tab of the mating piece.

8 The convex tabs on pieces 320-336, 516, 518 and 520 vary depending on
9 the atom(s) or group(s) to which the pieces 320-336, 516, 518 and 520 are
10 bound. Pieces 320-336 are designed to bind to at least one piece representing
11 an atom(s) or group(s) having one hydrogen. In this instance, the convex tab
12 347 would preferably have three flat sides generally in the shape of a square;
13 however, any shape can be used as long as it is consistent for the concavity of
14 the mating piece. The most common piece with convex tab 347 that each of
15 these pieces 320-336 is binding is the remaining half of the alkene molecule as
16 dissected by a vertical plane through the molecule, but may also be any other
17 piece representing an atom(s) or group(s) with a single hydrogen. Pieces 320-
18 336, 516, 518 and 520 can also contain convex tabs 349 where the piece is to
19 be bound to an atom(s) or group(s) having two hydrogens. Pieces 322, 324, and
20 516 have a convex tab 349 being generally in the shape of a triangle; however,
21 any shape can be used as long as it is consistent for the concavity of the mating
22 piece. Pieces 320-336, 516, 518 and 520 can also contain convex tabs 321

1 where the piece is to be bound to atom(s) or group(s) having three hydrogens.
2 Pieces 320, 326, and 518 have a convex tab 321 being generally in the shape of
3 a diamond; however, any shape can be used as long as it is consistent for the
4 concavity of the mating piece.

5 More specifically, piece 320 can bind to pieces 322, 323, and 330 due to
6 the square concavity and convex tabs present on one bonding side as well as
7 two other chemical fragments, one chemical fragment having one hydrogen
8 and the other chemical fragment having three hydrogens. This piece 320 along
9 with pieces 322, 323, 328, 330, and 332 are used to make vinyl groups.

10 Piece 322 can bind to pieces 320, 323, and 330 due to the square
11 concavity and convex tabs present on one bonding side as well as two other
12 chemical fragments, one chemical fragment having one hydrogen and the other
13 chemical fragment having two hydrogens.

14 Piece 323 can bind to pieces 320, 322, and 330 due to the square
15 concavity and convex tabs present on one bonding side as well as two other
16 chemical fragments each representative of a group having one hydrogen.

17 Piece 324 can bind to another alkene piece 320-336 due to the square
18 concavity and convex tabs present on one bonding side. The remaining bonding
19 side can bond a piece representing a chemical fragment having two hydrogens.

20 Piece 326 can bind to another alkene piece 320-336 due to the square
21 concavity and convex tabs present on one bonding side. The remaining bonding

1 side can bond a piece representing a chemical fragment having three
2 hydrogens.

3 Pieces 328 and 332 can bind to another alkene piece 320-336 due to the
4 square concavity and convex tabs present on one bonding side. The remaining
5 bonding side can bond a piece representing a chemical fragment having one
6 hydrogen.

7 Piece 330 can bond to pieces 320, 322, and 323 and can additionally
8 bond to a third group which does not observably split the hydrogen.

9 Pieces 334 and 336 can bind to another alkene piece 320-336 due to the
10 square concavity and convex tabs present on one bonding side. The remaining
11 bonding side can bond a piece representing a group that does not cause
12 observable splitting of the NMR peak.

13 Piece 516 can bind a piece representing an atom(s) or group(s) having
14 two hydrogens due to the triangular shaped convex tab 517 present on one
15 bonding side. The remaining bonding side 515 can bond a piece representing
16 an atom(s) or group(s) that does not cause observable splitting of the NMR
17 peak.

18 Piece 518 can bind a piece representing an atom(s) or group(s) having
19 three hydrogens due to the diamond shaped convex tab 519 present on one
20 bonding side. The remaining bonding side 515 can bond a piece representing
21 an atom(s) or group(s) that does not cause observable splitting of the NMR
22 peak.

1 The vinyl group pieces are represented by pieces 342, 502, 504, and 506.
2 Pieces 342 and 502-506 are shaped as a rectangle with three curved hydrogen
3 sides 343 and one bonding side 345. Bonding side 345 can be either flat 500 as
4 shown in piece 342 or contain concavities 501 and convex tabs 503, 505, and
5 507 as shown for pieces 502, 504, and 506 respectively. Where concavities and
6 convex tabs are present they indicate that these pieces would be bonded to an
7 atom(s) or group(s) that causes observable splitting of the NMR peak.

8 Piece 502 has a bonding side 345 that contains concavity 501 and convex
9 tab 503. Convex tab 503 is preferably shaped as a square; however, any shape
10 can be used as long as it is consistent for the concavity of the mating piece.
11 This piece 502 would be bonded to an atom(s) or group(s) having one hydrogen.

12 Piece 504 is designed to bond to an atom(s) or group(s) having two
13 hydrogens. Piece 504 has concavity 501 and convex tab 505. Convex tab 505 is
14 preferably shaped as an equilateral triangle; however, any shape can be used
15 as long as it is consistent for the concavity of the mating piece.

16 Piece 506 has a bonding side 345 that contains concavity 501 and convex
17 tab 507. Convex tab 507 is preferably shaped as a diamond; however, any
18 shape can be used as long as it is consistent for the concavity of the mating
19 piece. This piece 506 would be bonded to an atom(s) or group(s) having three
20 hydrogens.

21 Fig. 8a shows a top view of the benzene ring pieces 350-356 of the
22 present invention. The benzene ring pieces 350-356 are represented by a large

1 circle with one, two, three, four, five or six flat sides 358 representing mono-
2 through hexa-substituted benzene rings. The mono-substituted piece is
3 represented by piece 350. The relative position of the flat sides 358 indicates
4 the relative placement of the substituents around the ring. Piece 356
5 represents an ortho-arrangement of substituents having two flat sides 358 at
6 the ortho-position being 60 degrees apart. Piece 354 represents a meta-
7 arrangement of substituents having two flat sides 358 at the meta-position
8 being 120 degrees apart. Piece 352 represents a para-arrangement of
9 substituents having two flat sides 358 at the para-position being 180 degrees
10 apart. All flat sides 358 for benzene ring pieces 350-356 contain no
11 concavities or convex tabs. Additional pieces can easily be envisioned
12 representing the various tri-, tetra-, penta-, and hexa- substituted rings. The
13 present embodiment can also be extended to other aromatic and polycyclic
14 aromatic groups such as furan, naphthalene, pyridine, and the like.

15 Alternatively, Fig 8b shows the aromatic carbons of the benzene rings
16 represented as separate aromatic pieces 362-370, 382, and 384. These pieces
17 are preferably shaped as equilateral triangles. Flat sides 372 represent
18 bonding sides while curved sides 374 represent hydrogen sides. Piece 364 does
19 not have concavities and convex tabs which indicates that this piece would be
20 bonded to aromatic carbons or atoms without an attached hydrogen. Piece 362
21 has no attached hydrogens so it cannot split or be split by its neighbors. The

1 remaining pieces 366-370, 382 and 384 contain concavities and convex tabs on
2 the flat sides 372.

3 There is one type of concavity 376 present on pieces 366-370, 382, and
4 384 which has preferably two flat inset sides generally in the shape of a
5 triangle; however, any shape can be used as long as it is consistent on the
6 aromatic pieces. The convex tabs 378 used on the sides 380a and 380b are
7 generally triangular in shape; however, any shape can be used as long as it is
8 consistent with the concavity of the remaining aromatic pieces to which it is
9 bound. This scheme can be extended to include polycyclic aromatic rings.

10 In Fig. 9 a top view of the aldehyde pieces 390-396 of the present
11 invention is shown. The aldehyde pieces 390-396 have one flat side 398 and
12 one curved hydrogen side 400. One piece 390 is present without concavities
13 and convex tabs and would be bonded to an atom(s) or group(s) that does not
14 cause observable splitting of the NMR peak. The remaining pieces 392-396
15 contain concavities and convex tabs.

16 There is one type of concavity 402 present on pieces 392-396. This
17 concavity 402 has preferably three flat sides generally in the shape of a square;
18 however, any shape can be used as long as it is consistent on all aldehyde
19 pieces and the convex tabs of the mating pieces, including, but not limited to,
20 convex tabs 347, 312, 208, 236, 253, 158, 615 and 705. The convex tabs on the
21 aldehyde pieces 392-396 vary depending on the atom(s) or group(s) to which
22 the pieces can be bound.

1 When the atom(s) or group(s) to which pieces 392-396 can be bound has
2 one hydrogen, the convex tab 404 will preferably have three flat sides
3 generally in the shape of a square; however, any shape can be used as long as
4 it is consistent for the concavity of the mating piece. Piece 392 is capable of
5 binding to a mating piece representing an atom(s) or group(s) with one
6 hydrogen.

7 If the atom(s) or group(s) to which the piece 392-396 is bound has two
8 hydrogens, the convex tab 406 is preferably shaped as an equilateral triangle;
9 however, any shape can be used as long as it is consistent for the concavity of
10 the mating piece. Piece 394 is capable of binding to a mating piece
11 representing an atom(s) or group(s) with two hydrogens.

12 In addition, when the atom(s) or group(s) to which the piece 392-396 is
13 bound has three hydrogens, the convex tab 408 is preferably shaped as a
14 diamond; however, any shape can be used as long as it is consistent for the
15 concavity of the mating atom(s) or group(s). Piece 396 can bind to a piece
16 representing an atom(s) or group(s) with three hydrogens.

17 Fig. 10 is a top view of the ketone group pieces 416-420 of the present
18 invention. The ketone group pieces 416-420 include standard ketone piece
19 416, the ether piece 418, and carboxyl group 420. All ketone group pieces 416-
20 420 are rectangular with two flat sides 417 and two curved ends 419. All
21 pieces are present without concavities and convex tabs. Other pieces that can
22 be included in this group with the same overall characteristics include, but are

1 not limited to, anhydrides, ethers, esters, sulfides, sulfoxides, sulfones, and
2 alkynes.

3 In Fig. 11 a top view of the halide piece 422 of the present invention is
4 shown. Piece 422 has one bonding side 800 and one curved side 802. This
5 piece 422 is present without concavities and convex tabs since the halides do
6 not cause observable splitting of the NMR peak. Other pieces that can be
7 included in this group with the same overall characteristics include, but are not
8 limited to, pieces for cyano and azide groups (not shown).

9 Fig. 12 is a top view of a base methyl piece 600 of another embodiment
10 of the present invention with interchangeable tabs 602, 614 and 618. Base
11 methyl piece 600 has a cavity defined by portions 601, 606, and 608. This
12 cavity is designed to accept interchangeable tabs 602, 614 and 618 allowing a
13 snug fit of portions 610, 607, and 609 of interchangeable tabs 602, 614 and 618
14 against portions 601, 606, and 608 of base methyl piece 600 respectively to
15 form the final piece 605. A locking mechanism (not shown) may also be
16 provided.

17 Final piece 605 could then substitute for piece 220 in the preferred
18 embodiment where interchangeable tab 602 has a diamond shaped concavity
19 603 and triangular shaped convex tab 604. Any other shape can be substituted
20 for the concavity 603 and convex tab 604 on interchangeable tab 602 as long as
21 the concavity 603 is consistent for all methyl pieces and the convex tab 604 is
22 consistent for the concavity of the mating piece.

1 Where final piece 605 incorporates interchangeable tab 618 having a flat
2 bonding side 616, it could substitute for piece 216 in the preferred
3 embodiment.

4 Final piece 605 could also substitute for piece 218 in the preferred
5 embodiment where interchangeable tab 614 is used having a diamond shaped
6 concavity 603 and a square convex tab 615. Any shape can be substituted for
7 the concavity 603 and the convex tab 615 on interchangeable tab 614 as long as
8 the concavity 603 is consistent for all methyl pieces and the convex tab 615 is
9 consistent for the concavity of the mating piece.

10 For purposes of this example, the base piece was selected as a methyl
11 piece; however, any other disclosed piece could be substituted as the base
12 piece with one or more cavities defined by portions 601, 606, and 608 that can
13 accept interchangeable tabs defined by the respective concavities and convex
14 tabs provided on the disclosed pieces herein.

15 Fig. 13 is a perspective view of another embodiment of the present
16 invention showing a base methyl piece 700 with a single rotating tab member
17 704. Base methyl piece 700 has a cavity defined by portions 701, 702, and 703.
18 This cavity accommodates rotating tab member 704 providing for attachment
19 points (not shown) for portion 711 of rotating tab member 704 to attach to
20 portion 701 of base methyl piece 700 and for portion 710 of rotating tab
21 member 704 to attach to portion 703 of base methyl piece 700. Rotating tab
22 member 704 has four sides each defining a different bonding environment for

1 the base methyl piece 700. Where the base methyl piece 704 is to be bonded
2 to an atom(s) or group(s) that does not cause observable splitting of the NMR
3 peak, flat side 709 would be rotated 180 degrees to the outside or exposed
4 bonding edge to form the final piece which could be substituted for piece 216.

5 Where the base methyl piece 700 is to be bonded to an atom(s) or
6 group(s) that cause observable splitting of the NMR peak and this atom(s) or
7 group(s) has only one hydrogen, such as a methine piece, side 715 of the
8 rotating tab member 704 can then be rotated if necessary (however in Fig. 13
9 it is already on the exposed bonding edge) to form the final piece which could
10 substitute for piece 218. Here convex tab 705 is square shaped and concavity
11 706 is diamond shaped. However, any shape can be substituted for the
12 concavity 706 and the convex tab 705 as long as the concavity 706 is consistent
13 for all methyl pieces and the convex tab 705 is consistent for the concavity of
14 the mating piece.

15 Where the base methyl piece 700 is to be bonded to an atom(s) or
16 group(s) that cause observable splitting of the NMR peak and this atom(s) or
17 group(s) has two hydrogens, such as a methylene piece, side 716 of the rotating
18 tab member 704 can then be rotated 90 degrees to form the final piece which
19 could substitute for piece 220. Here convex tab 717 is triangular shaped and
20 concavity 707 is diamond shaped. However, any shape can be substituted for
21 the concavity 707 and the convex tab 717 as long as the concavity 707 is.

1 consistent for all methyl pieces and the convex tab 717 is consistent for the
2 concavity of the mating piece.

3 The last side (not shown) will be used where the piece is to be bonded
4 to an atom(s) or group(s) that cause observable splitting of the NMR peak and
5 this atom(s) or group(s) has three hydrogens. For the base methyl piece 700
6 this portion of the rotating tab member 704 will not be included as such a bond
7 would create ethane which is a singlet in the NMR spectrum. For other pieces
8 it can be included. This last side can be rotated to form the final piece. Here
9 both the concavity and convex tab would be shaped as a diamond. However,
10 any shape could be used as long as the concavity is consistent for all methyl
11 pieces and the convex tab is consistent for the concavity of all mating pieces.

12 For this example, a methyl piece was used as the base piece; however,
13 any disclosed piece could be substituted as the base piece with one or more
14 cavities defined by portions 701, 702, and 703 that can accept the rotating tab
15 member 704 having one flat side and three sides defined by the respective
16 concavities and convex tabs provided on the pieces disclosed herein. The
17 distance from the end of one convex tab to the end of the opposing convex tab
18 located 180 degrees apart will be no greater than the thickness of the base
19 piece. A gap will be provided between portion 702 of the base piece and the
20 rotating tab member 704 to allow free rotation of the rotating tab member. A
21 locking mechanism (not shown) may be provided.

1 These pieces described in Figs. 1-13, along with the tested methodology,
2 simplify NMR structural analysis for students. The students analyze each signal
3 to determine all information present in the spectrum. During this analysis, the
4 students determine each anticipated chemical fragment from the shift on the
5 NMR spectrum based on the standard chemical shifts known for various
6 chemical fragments. In addition, the students determine the splitting from the
7 spectrum to determine the number of hydrogen neighbors that exist for a
8 particular hydrogen or group of equivalent hydrogens. Last in the analysis is
9 integration which gives the students information on the number of hydrogens
10 that a given resonance represents on the NMR spectrum.

11 The analysis results in the students determining the applicable pieces of
12 the unknown molecule. Once the pieces are known, the pieces can be put
13 together to form the unknown molecule. Due to the interlocking nature of the
14 pieces, the students are not able to manipulate the pieces to force them into a
15 structure that is not consistent with the spectrum information provided. From
16 experiments using the present NMR teaching method and apparatus, students
17 were found to solve NMR structures in half the time compared to students who
18 did not have the present invention. Some examples are illustrative.

1 **EXAMPLE 1:**2 **1. ^1H NMR Spectrum for Unknown Molecule $\text{C}_2\text{H}_5\text{Br}$ is incorporated herein by**
3 **reference.**

4

5

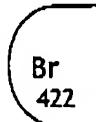
6 **2. Using the Present Invention:**7 **Peak integration is 2:3. Peak at 3.4δ is a CH_2 (from chemical shift and**
8 **integration), but is next to an electronegative atom Br due to the chemical**
9 **shift. Pull the halide chemical fragment piece.**

10

11

12

13



14

15

16

17 **The peak at 3.4δ is also a quartet which indicates there are three**18 **adjacent neighbor hydrogens. Pull a CH_2 piece that can bind to a group**19 **representing three hydrogens, i.e., one having a diamond convex tab.**

20

21

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26 **The peak at 1.7δ is a CH_3 (from chemical shift and integration) and the**27 **triplet indicates an adjacent two hydrogens. Choose a CH_3 piece that can bind**28 **to a group representing two hydrogens, i.e., one having a triangular convex**

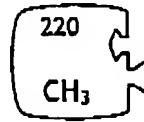
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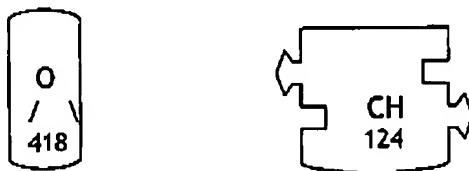
**3. Solving for the Unknown Molecule**

1 The pieces may then be put together to form the molecule ethyl
2 bromide C₂H₅Br:

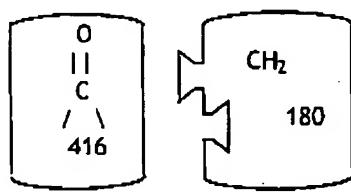


1 2. Using the Present Invention:
2
3

4 There is a heptet at 5.0δ having one hydrogen (from integration). Begin
5 to look for a CH piece. The chemical shift indicates this component is next to
6 an oxygen. Choose an oxygen piece. The splitting into the heptet indicates this
7 component is next to six neighbor hydrogens. Choose a CH piece that can bind
to six hydrogens i.e. two methyl groups.

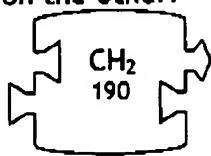


8
9
10
11
12
13
14 There is a triplet at 2.2δ which has two hydrogens (from integration).
15 Begin looking at the CH_2 pieces. The chemical shift indicates this component is
16 next to a carbonyl. Select a ketone piece. The triplet indicates this
17 component is next to two neighbor hydrogens. Select a CH_2 piece which can
18 bind to a component having two hydrogens i.e. a piece having the triangular
19 convex tab.



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21
22
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26
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28
29 There is a hextet at 1.6δ having two hydrogens (from integration). The
chemical shift indicates an alkyl group. The hextet indicates this component
is next to five neighbor hydrogens, three on one side, and two on the other.

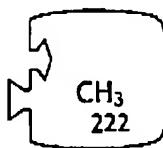
- 1 Select the appropriate CH_2 piece having a triangular convex tab on one side
2 and a diamond convex tab on the other.



3
4
5
6 There is a doublet at 1.2δ with six hydrogens (from integration). The
7 chemical shift indicates it is an alkyl group. The doublet indicates it's next to
8 one neighbor hydrogen. This must represent two equivalent CH_3 groups (since
9 six hydrogens are involved) each next to a component having one hydrogen i.e.
10 next to a component having a square convex tab. Select two CH_3 pieces having
11 a square convex tab.

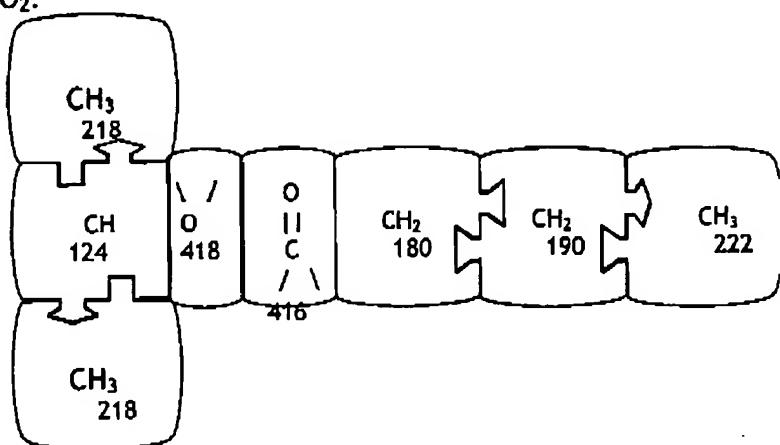


12
13
14
15
16 There is a triplet at 0.9δ having three hydrogens (from integration).
17 The chemical shift indicates it's an alkyl group. The triplet indicates this group
18 is next to two neighbor hydrogens. Select a CH_3 piece with a triangular convex
19 tab representing the neighboring component with two hydrogens.



1 3. Solving for the Unknown Molecule:

2 Assemble pieces, making sure to use all pieces and take into account
3 chemical shift information. The pieces can be put together to form isopropyl
4 butyrate, C₇H₁₄O₂.



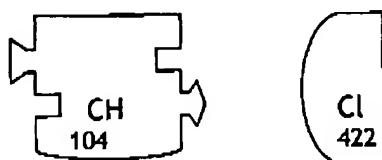
21 EXAMPLE 3:

22 1. ¹H NMR Spectrum for Unknown Molecule C₄H₉Cl is incorporated herein by
23 reference.

24
25
26
27 While this spectrum has fewer peaks than EXAMPLE 2, it is frequently
28 more difficult for students due to the complex multiplet signal at 1.75 δ.
29 Students often feel that this makes the spectrum impossible since one cannot
30 determine the number of hydrogens adjacent to this hydrogen.

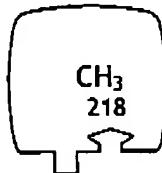
36 2. Using the Present Invention:

1 There is a hextet at 4.0δ that has one hydrogen (from integration). The
2 chemical shift indicates this group is adjacent to an electronegative Cl. Select
3 a Cl piece. The hextet indicates this group is also next to five neighbor
4 hydrogens. Select a CH piece that can bind to five hydrogens i.e. a CH piece
5 having two different convex tabs-one that can bind to two hydrogens
6 (triangular convex tab) and one that can bind to three hydrogens (diamond
7 convex tab).



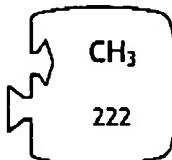
13 There is a multiplet at 1.75δ that has two hydrogens (from integration).
14 Begin looking at the alkyl CH_2 pieces, but at this point one cannot tell about
15 the neighbor hydrogens other than there are several.

16 There is a doublet at 1.5δ which has three hydrogens. The chemical
17 shift indicates it is an alkyl group while the doublet indicates this group is next
18 to one neighbor hydrogen. Select a CH_3 piece that has a square convex tab.



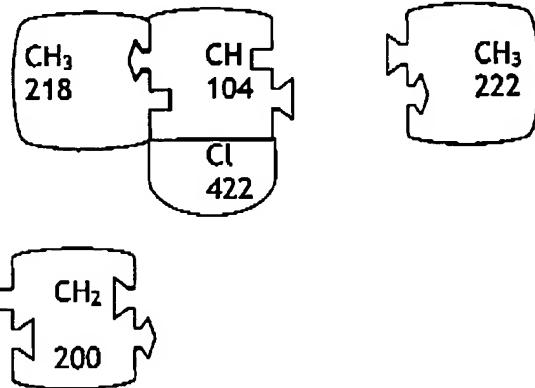
24 There is a triplet at 1.0δ that has three hydrogens. The chemical shift
25 indicates it is an alkyl group. The triplet indicates that it is next to two

1 neighbor hydrogens. Select a CH_3 piece having a triangular convex tab
2 representative of a neighboring component having two hydrogens.

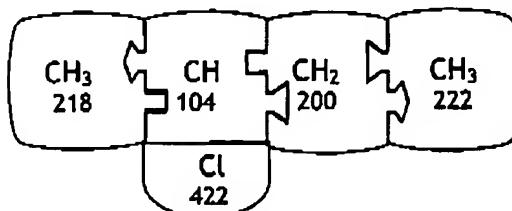


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4
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8
9 3. Solving for the Unknown Molecule:

10
11 Put the known pieces together. Notice that once the known pieces are
12 assembled the undetermined CH_2 piece is obvious from the neighbor pieces
13 which must bond to it as follows:



24
25
26
27
28
29 Undetermined CH_2 piece



1 The final structure is therefore determined to be *sec*-butyl chloride,
2
3 C₄H₉Cl.

4 EXAMPLE 4:

5 1. ^1H NMR Spectrum for Unknown Molecule $\text{C}_{13}\text{H}_{16}\text{O}_3$ is incorporated here in by
6 reference.
7

8 This spectrum is very complex. Such spectra are typically solved along
9
10 with Infrared Spectra which help determine which chemical fragments are
11 present in the molecule. This molecule is extremely difficult to identify using
12 the "look, see, guess" method in which students solve the spectrum by
13 guessing chemical structures. Using this approach there are two recognizable
14 groups: a di-substituted aromatic ring at $6.8\text{-}7.8\delta$, and an isolated ethyl group
15 at 2.5δ , 1.0δ . Further analysis using the present invention, however,
16 demonstrates that the quartet/triplet pattern of the ethyl group is in fact not
17 correct. This molecule has no isolated ethyl group. Such misidentifications
18 using the "look, see, guess" method are a common occurrence in complex
19 spectra such as this and make the "look, see, guess" method a very poor
20 approach for solving complex spectra.

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7 2. Using the Present Invention:

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9 Initial analysis of the NMR and IR data are similar in both existing
10 methods and the method of the present invention. The band at 10.8 δ could be
11 either a carboxylic acid or phenol. Analysis of the liquid thin film infrared
12 spectrum indicates it is a phenol due to the lack of extensive OH hydrogen
13 bonding at 2500- 3300 cm^{-1} .

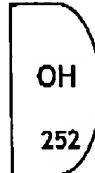
14 Acyclic alkanes have the general formula C_nH_{2n+2} while cyclic alkanes and
15 alkenes have the generally formula C_nH_{2n} . The degree of unsaturation of the
16 molecule is calculated by determining the number of hydrogens for the
17 corresponding saturated alkane and subtracting the number of hydrogens
18 actually present and dividing by two. The present molecule has thirteen
19 carbons so the number of hydrogens for the corresponding saturated alkane
20 would be $(2n+2)$ or 28. Oxygen atoms are ignored. Subtracting out the number
21 of hydrogens actually present (16) means there are twelve hydrogens missing
22 compared to a totally saturated molecules.

23 The degree of unsaturation is determined by dividing this number by
24 two. This indicates there are $12/2 = 6$ double bonds and/or rings in the
25 molecule. The NMR and IR indicate the presence of an aromatic ring (4
26 unsaturations), a carbonyl group (1 unsaturation); thus the two alkene

1 hydrogens observed in the NMR must be on a single double bond (1
2 unsaturation). Finally the combination of three oxygens in the molecule, the
3 presence of a phenol and carbonyl (IR at 1680 cm^{-1}) and the strong IR bands at
4 $1200\text{-}1300\text{ cm}^{-1}$ indicate that the molecule contains an ester functionality.
5 Select the ester piece 420.

6 2. Using the Present Invention:

7 There is a singlet at 10.8δ with one hydrogen (from integration). This is
8 due to a carboxylic acid or alcohol (phenol). Analysis of the liquid thin film
9 infrared spectrum indicates it is a phenol due to the lack of extensive OH
10 hydrogen bonding at $2500\text{-}3300\text{ cm}^{-1}$. Select an OH piece.



23 There is a doublet at 7.8δ with one hydrogen (from integration). This is
24 an aromatic hydrogen with one neighbor hydrogen. Select an aromatic piece
25 having one neighbor hydrogen i.e. having one triangular concavity and one
26 triangular convex tab.



30 There is a triplet at 7.4δ with one hydrogen (from integration). This is
31 an aromatic hydrogen with two neighbor hydrogens. Select an aromatic piece
32 with two sets of triangular concavities and convex tabs.

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There is a doublet at 7.0δ with one hydrogen (from integration). This is another aromatic hydrogen with one neighbor hydrogen. Select another

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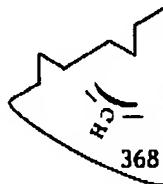
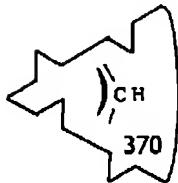
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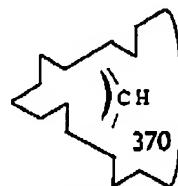
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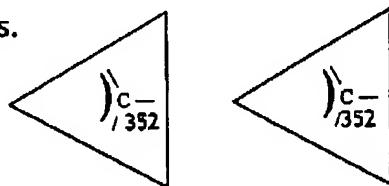
There is a doublet at 7.0δ with one hydrogen (from integration). This is another aromatic hydrogen with one neighbor hydrogen. Select another aromatic piece with one triangular concavity and one triangular convex tab.

There is a triplet at 6.8δ with one hydrogen (from integration). This is another aromatic hydrogen with two neighbor hydrogens. Select an aromatic piece

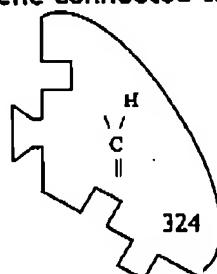
1 with two sets of triangular concavities and convex tabs.



The presence of only four aromatic hydrogens indicates that there are two aromatic carbons without any attached hydrogens. The pieces below represent such pieces.



There is a quartet at 5.6δ with long range splitting having one hydrogen. This is an alkene hydrogen with three neighbor hydrogens. Since there are two alkene hydrogens (see the 5.4δ peak) and a single alkene double bond, this must be a di-substituted alkene connected to a CH_2 group. The piece below represents such a piece.



There is a quartet at 5.4δ with long range splitting having one hydrogen. This is an alkene hydrogen with three neighbor hydrogens. Since there are two alkene hydrogens (see the 5.6δ peak) and a single alkene double bond, this must be a di-substituted alkene connected to a CH_2 group. The piece below represents such

1 a piece.

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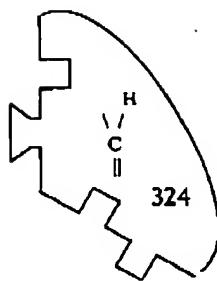
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9 There is a triplet at 4.3δ with two hydrogens (from integration). The
10 chemical shift indicates that these two hydrogens are adjacent to an oxygen.
11 The triplet splitting indicates this group has two neighbor hydrogens. Select a
12 CH_2 piece with a triangular convex tab for connection to a piece having two
13 hydrogens.

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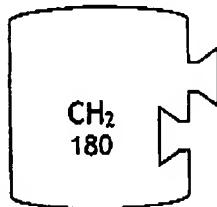
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21 There is a quartet at 2.5δ having two hydrogens (from integration). The
22 chemical shift indicates that these two hydrogens are adjacent to a carbonyl or
23 alkene. The quartet splitting indicates this group is next to three neighbor
24 hydrogens. Select a CH_2 piece having a diamond convex tab for connection to a
25 piece having three hydrogens.

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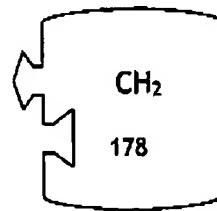
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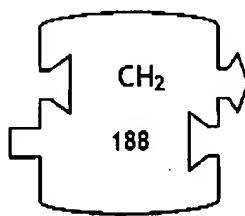
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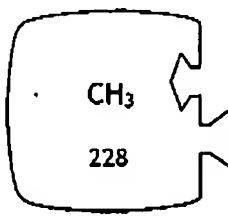
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1
2 There is a pentet at 2.1 δ having two hydrogens (from integration). The
3 chemical shift indicates that these two hydrogens are adjacent to a carbonyl or
4 alkene. The pentet indicates that the present group is next to four neighbor
5 hydrogens. Since there are four neighbor hydrogens, it is impossible for the
6 group to be next to a carbonyl, so it must be next to the alkene. Select a CH₂
7 piece having a square convex tab for connection to a piece having one
8 hydrogen and a diamond convex tab for connection to a piece having three
9 hydrogens.

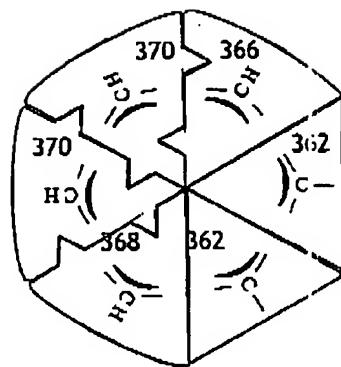


17
18 There is a triplet at 1.0 δ having three hydrogens (from integration). The
19 chemical shift indicates these three hydrogens are on an alkyl group. The
20 triplet indicates that this component has two neighbor hydrogens. Select a CH₃
21 piece having a triangular convex tab representative of a component having two
22 hydrogens.



1 3. Solving for the Unknown Molecule:
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a) Aromatic ring:



1 There are problems in the first attempt to put the molecule together.
2 See Fig. 14A. There are two pieces which can bond to the piece 228 and no
3 part to connect the alkene and aromatic chemical fragments. This indicates
4 that the splitting has been misinterpreted. There is not an isolated ethy.
5 group. The methylene quartet at 2.5 δ must not be adjacent to a methyl, but
6 rather two hydrogens on one side and a single hydrogen on the other.
7 Replacement of piece 178 with piece 176 allows completion of the molecule.
8 See Fig. 14B.

9 In accordance with the principles of the present invention, the
10 functionality disclosed herein can not only be implemented manually, but can
11 be implemented by hardware, software, and/or a combination of both.
12 Software implementations can be written in any suitable language or a
13 combination of languages where applicable, including fourth generation
14 languages defined as programming languages closer to human languages than
15 typical high level (third generation) programming languages. Most fourth
16 generation languages are used to access databases. The software
17 implementation can also be written in a third generation languages such as,
18 but not limited to, Ada, Algol, BASIC, COBOL, C, C++, FORTRAN, LISP, Pascal,
19 and Prolog. These third generation languages are known as high level
20 programming languages and are defined as enabling a programmer to write
21 programs that are more or less independent of a particular type of computer.

1 These languages are considered high-level because they are closer to human
2 languages and further from machine languages.

3 The software used in the invention can also be written in a second
4 generation language or assembly language. Assembly language is a
5 programming language once removed from a computer's machine language.
6 This language has the same structure and set of commands as machine
7 languages, but enables a programmer to use names instead of numbers.

8 It is rare, but possible that the present software will incorporate first
9 generation language or machine language. Machine language is the only
10 language understood by computers. While easily understood by computers,
11 machine languages are almost impossible for humans to use because they
12 consist entirely of numbers. Programs written in high-level languages are
13 translated into assembly language or machine language with a compiler or
14 interpreter. Assembly language programs are translated into machine language
15 with an assembler program.

16 The system running such a software program would have a standard
17 computer subsystem, such as the IBM personal computer (also known as the IBM
18 PC), including a CPU (e.g. a microcomputer system, including a central
19 processing unit, disk drive, etc.), a display device (such as a standard CRT
20 monitor or television monitor), an input device (such as a keyboard or mouse),
21 an application specific piece of hardware, or other suitable device. It is
22 preferred that the computer subsystem incorporate a graphical user interface

1 operating system such as, but not limited to, Mac OS/System, UNIX or
2 Windows. Additional functions that are preferred, but not required from the
3 operating system include multi-user capability, multiprocessing, multitasking,
4 and multithreading.

5 In addition to using discrete hardware components in a logic circuit, the
6 required logic may also be performed by an application specific integrated
7 circuit ("ASIC"), a programmed programmable logic device ("PLD"), or other
8 device. The system will also include various hardware components which are
9 well known in the art, such as connectors, cables, and the like. Moreover, at
10 least part of this functionality may be embodied in computer readable media
11 (also referred to as computer program products), such as magnetic, magnetic-
12 optical, and optical media, used in programming an information-processing
13 apparatus to perform in accordance with the invention. This functionality also
14 may be embodied in computer readable media, or computer program products,
15 such as a transmitted waveform to be used in transmitting the information or
16 functionality.

17 The software/ hardware program of the present invention can include a
18 student tutorial application and/or a laboratory identification application. In
19 both applications, a series of user interface screens will be displayed. These
20 screens illustrate what the user sees when participating in the student tutorial
21 application or laboratory identification application respectively. It will of
22 course be understood that the application of the present invention to a

1 software or hardware program is not restricted to the particular user interfaces
2 illustrated. Rather, any suitable user interface can be employed.

3 The student tutorial application will be discussed first. In the student
4 tutorial application, the initial configuration screen will appear which includes
5 a plurality of check boxes or the like through which the student user can select
6 which application functions he or she wishes to explore. These check boxes are
7 selected and deselected by selective mouse clicks. The actual items listed on
8 the configuration screen correspond to application functions specific to the
9 program, such as, but not limited to skill level, molecule type, and random
10 sort.

11 After the student user has selected the desired functions, the OK button
12 on the screen is clicked, whereupon the chosen testing sequence begins. The
13 testing sequence begins in the next window, the selection screen, which
14 provides an NMR spectrum. The student user is then prompted at the selection
15 screen to select atoms or groups from the screen to begin the identification.
16 These atoms and groups are labeled on descriptive buttons provided on the
17 screen. These atom and group buttons are selected and deselected by
18 selective mouse clicks. Upon each selection of the atom or group, the
19 respective atom or group appears on the screen as a larger and moveable
20 component on the screen.

21 When the student user has selected all atoms and/or groups he or she
22 believes are applicable, the OK button on the screen is clicked. The student

1 user is then prompted in the arrangement screen to select between buttons
2 that display such functions as auto-arrange and manual arrange. These buttons
3 are selected by mouse clicks. Upon selection of auto-arrange, the selected
4 atom and/or group pieces are automatically arranged on the computer screen
5 to provide the best fit or a series of applicable fits between the chosen atom
6 and/or group pieces. Selection of manual arrange simply allows the student
7 user to move the atom and/or group pieces on the screen himself to obtain a
8 perfect fit. If a perfect fit cannot be found, the student user will be prompted
9 to return to the selection screen to try again, to try another molecule, or to
10 see the answer.

11 If a perfect fit is found between the chosen atom and/or group pieces,
12 an exclamation on the screen will appear such as, but not limited to, "Perfect
13 Fit". If a perfect fit is found, the student user is then prompted by an open
14 box to write the name of the unknown molecule. If the name keyed into the
15 open box by the student user is the identity of the unknown molecule, an
16 exclamation will appear on the screen, such as, but not limited to,
17 "Congratulations, you've identified the unknown molecule". The student user
18 can then be prompted to select between buttons that display functions such as,
19 but not limited to, "Try Another", "View 3D", and "View MSDS". These
20 buttons are selected by mouse clicks.

21 If the name keyed into the open box by the student user is not the
22 identity of the unknown molecule, an exclamation will appear on the screen

1 such as, but not limited to, "Oops, try again". The student user will then be
2 returned to the selection screen and prompted to select between buttons that
3 allow the student user to decide whether to change the existing selection or
4 start a new selection of atoms and/or groups. The buttons are selected by
5 mouse clicks. Once the student user has entered the new atoms and/or
6 groups, again the student user can choose to auto arrange the pieces in the
7 arrangement screen and determine if a perfect fit exists. The student user can
8 again type in the applicable name to determine if he or she has correctly
9 identified the molecule.

10 The application can be preconfigured at the configuration screen to
11 repeat continuously until the right answer is obtained or to repeat for only a
12 pre-designated number of times before the student user is prompted with the
13 correct identification and atom and/or group arrangement of the unknown
14 molecule. With each wrong name entered, the student user will be prompted
15 to select between buttons that display functions such as, but not limited to,
16 "Try Another" and "See Answer". These buttons can be selected by mouse
17 clicks.

18 The laboratory identification application can exist independently, with
19 the student tutorial application or associated with the computer system of an
20 NMR instrument in a laboratory. In the laboratory identification application, an
21 initial configuration screen will appear which includes a plurality of checkboxes
22 or the like through which the laboratory user can select which application

1 functions he or she wishes to explore. The check boxes are selected and
2 deselected by selective mouse clicks. The actual items listed on the
3 configuration screen correspond to application functions specific to the
4 program, such as, but not limited to scan spectrum, run spectrum and enter
5 peaks.

6 After the laboratory user has selected the desired functions, the OK
7 button is clicked on the screen, whereupon the chosen function begins. The
8 scan spectrum function begins in the next window which shows the NMR
9 spectrum image being scanned onto the screen from a paper copy. The
10 spectrum could also be transferred directly from the spectrometer acquisition
11 program. The laboratory user is then prompted with various formatting
12 functions such as clarifying the image. Once the desired image is obtained
13 from the formatting, the laboratory user can then select a button on the screen
14 such as "Accept Image".

15 Once the laboratory user has accepted the NMR spectrum image from
16 the paper scan, the laboratory user is then prompted at a selection screen to
17 select atoms and/or groups from the screen to begin identification. These
18 atoms and groups are labeled as descriptive buttons provided on the screen.
19 These atom and group buttons are selected and deselected by selective mouse
20 clicks. Upon each selection of the atom or group, the respective atom or group
21 appears on the screen as a larger and moveable component on the screen.

1 When the laboratory user has selected all atoms and/or groups he or she
2 believes are applicable, the OK button on the screen is clicked. The laboratory
3 user is then prompted in the arrangement screen to select between buttons
4 that display such functions as auto arrange and manual arrange. These buttons
5 are selected by mouse clicks. Upon selection of auto-arrange, the selected
6 atom and/or group pieces are automatically arranged on the computer screen
7 to provide the best fit or series of applicable fits between the chosen atom
8 and/or group pieces. Selection of manual arrange simply allows the laboratory
9 user to move the atom and/or group pieces on the screen himself to obtain a
10 perfect fit. If a perfect fit cannot be found, the laboratory user will be
11 prompted to return to the selection screen to try again or to access the built in
12 NMR spectrum database to obtain the identity of the molecule or a series of
13 possible identities by randomly choosing suspected possibilities.

14 If a perfect fit is found between the chosen chemical fragment pieces,
15 an exclamation on the screen will appear such as, but not limited to, "Perfect
16 Fit". If a perfect fit is found, the laboratory user is then prompted by an open
17 box to write the name of the unknown molecule. A button is also provided on
18 the screen that upon selection by the laboratory user allows the program to
19 automatically provide a name for the unknown molecule or a list of
20 possibilities. Once the name is entered by either means, the program will then
21 search within the built in NMR spectrum database to determine if a spectrum
22 for the suspected molecule is contained therein. If one exists, the NMR

1 spectrum will be displayed on the screen in the same window as the scanned
2 NMR spectrum image so the laboratory user or the program can perform a
3 comparison of the spectra. The laboratory user can then be prompted to select
4 between buttons that display functions such as, but not limited to, "Scan
5 Another", "View 3D", and "View MSDS". These buttons are selected by mouse
6 clicks.

7 If the laboratory user is not satisfied with the search results, the
8 laboratory user can select from buttons on the screen that prompt the
9 laboratory user to return to the selection screen to try again with a new
10 selection of atoms and/or groups or to access the built in NMR spectrum
11 database to obtain the identity of the molecule or a series of possible identities
12 by randomly choosing suspected possibilities. Alternatively, the program may
13 search the database to find similar spectra by matching the peaks. This is
14 common in commercial infrared and mass spectrometer instruments. The
15 laboratory user can also return to the open box and type in names similar to
16 the suspected name of the unknown molecule.

17 If the laboratory user decides to try again at the selection screen, the
18 laboratory user will again enter possible atoms and/or groups. Once the
19 laboratory user has entered the new atoms and/or groups, again the laboratory
20 user can choose to auto arrange the pieces in the arrangement screen and
21 determine if a perfect fit exists. The laboratory user can again type in the

1 applicable name to access an NMR spectrum from the built in NMR spectrum
2 database.

3 When a laboratory user selects the run spectrum function, the
4 application launches into the applicable software program provided with the
5 NMR instrument from the manufacturer and/or supplier of NMR spectrometers.
6 Since the laboratory user will be interfaced into this second software program,
7 the screens that appear from this point in this second software program are the
8 proprietary materials of those respective companies.

9 When a laboratory user selects the enter peaks function button, this
10 function is launched onto the screen prompting the laboratory user to enter the
11 chemical shift for peaks on the NMR spectrum, integration if known, and the
12 splitting. Once the laboratory user has entered the peak information, a cursory
13 NMR spectrum will appear on the screen. The laboratory user is prompted with
14 buttons to select whether this NMR spectrum is correct. The buttons are
15 selected by mouse clicks.

16 Once the laboratory user has approved the NMR spectrum on the screen,
17 the laboratory user is then prompted at a selection screen to select atoms
18 and/or groups from the screen to begin identification. These atoms and groups
19 are labeled as descriptive buttons provided on the screen. These atom and
20 group buttons are selected and deselected by selective mouse clicks. Upon
21 each selection of the atom or group, the respective atom or group appears on
22 the screen as a larger and moveable component on the screen.

1 When the laboratory user has selected all atoms and/or groups he or she
2 believes are applicable, the OK button on the screen is clicked. The laboratory
3 user is then prompted in the arrangement screen to select between buttons
4 that display such functions as auto arrange and manual arrange. These buttons
5 are selected by mouse clicks. Upon selection of auto-arrange, the selected
6 atom and/or group pieces are automatically arranged on the computer screen
7 to provide the best fit or series of applicable fits between the chosen atom
8 and/or group pieces. Selection of manual arrange simply allows the laboratory
9 user to move the atom and/or group pieces on the screen himself to obtain a
10 perfect fit. If a perfect fit cannot be found, the laboratory user will be
11 prompted to return to the selection screen to try again or to access the built in
12 NMR spectrum database to obtain the identity of the molecule or series of
13 possible identities by randomly choosing suspected possibilities.

14 If a perfect fit is found between the chosen atom and/or group pieces,
15 an exclamation on the screen will appear such as, but not limited to, "Perfect
16 Fit". If a perfect fit is found, the laboratory user is then prompted by an open
17 box to write the name of the unknown molecule. A button is also provided on
18 the screen that upon selection by the laboratory user allows the program to
19 automatically provide a name for the unknown molecule or a list of
20 possibilities. Once the name is entered by either means, the program will then
21 search within the built in NMR spectrum database to determine if a spectrum
22 for the suspected molecule is contained therein. If one exists, the NMR

1 spectrum will be displayed on the screen in the same window as the cursory
2 image so the laboratory user or the program can perform a comparison of the
3 spectra. The laboratory user can then be prompted to select between buttons
4 that display functions such as, but not limited to, "Enter Another", "View 3D",
5 and "View MSDS". These buttons are selected by mouse clicks.

6 If the laboratory user is not satisfied with the search results, the
7 laboratory user can select from buttons on the screen that prompt the
8 laboratory user to return to the selection screen to try again with a new
9 selection of atoms and/or groups or to access the built in NMR spectrum
10 database to obtain the identity of the molecule or a series of possible identities
11 by randomly choosing suspected possibilities. The laboratory user can also
12 return to the open box and type in names similar to the suspected name of the
13 unknown molecule.

14 If the laboratory user decides to try again at the selection screen, the
15 laboratory user will again enter possible atoms and/or groups. Once the
16 laboratory user has entered the new atoms and/or groups, again the laboratory
17 user can choose to auto arrange the pieces in the arrangement screen and
18 determine if a perfect fit exists. The laboratory user can again type in the
19 applicable name to access an NMR spectrum from the built in NMR spectrum
20 database.

1 If the name is not found in the NMR spectrum database, the user will be
2 notified and any final structural identification will be limited to the
3 identification found during the "Perfect Fit".

4 Although the invention has been described with reference to specific
5 embodiments, this description is not meant to be construed in a limited
6 sense. Various modifications of the disclosed embodiments, as well as
7 alternative embodiments of the inventions will become apparent to persons
8 skilled in the art upon the reference to the description of the invention.
9 Accordingly it is intended to embrace all such alternatives, modifications and
10 variations as fall within the spirit and broad scope of the invention. It is,
11 therefore, contemplated that the appended claims will cover such
12 modifications that fall within the scope of the invention.